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Advanced Nuclear Energy Analysis Technology

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ADVANCED NUCLEAR ENERGY ANALYSIS TECHNOLOGY

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Abstract

A two-year effort focused on applying ASCI technology developed for the analysis of weapons systems to the state-of-the-art accident analysis of a nuclear reactor system was proposed. The Sandia SIERRA parallel computing platform for ASCI codes includes high-fidelity thermal, fluids, and structural codes whose coupling through SIERRA can be specifically tailored to the particular problem at hand to analyze complex multiphysics problems. Presently, however, the suite lacks several physics modules unique to the analysis of nuclear reactors. The NRC MELCOR code, not presently part of SIERRA, was developed to analyze severe accidents in present-technology reactor systems. We attempted to: 1) evaluate the SIERRA code suite for its current applicability to the analysis of next generation nuclear reactors, and the feasibility of implementing MELCOR models into the SIERRA suite, 2) examine the possibility of augmenting ASCI codes or alternatives by coupling to the MELCOR code, or

portions thereof, to address physics particular to nuclear reactor issues, especially those facing next generation reactor designs, and 3) apply the coupled code set to a demonstration problem involving a nuclear reactor system.

We were successful in completing the first two in sufficient detail to determine that an extensive demonstration problem was not feasible at this time. In the future, completion of this research would demonstrate the feasibility of performing high fidelity and rapid analyses of safety and design issues needed to support the development of next generation power reactor systems.

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1. INTRODUCTION

After nearly 20 years with no clear national energy policy, our nation is in the process of articulating an energy plan for the foreseeable future, motivated by emerging issues of national and indeed global importance. These issues include acute electrical energy production shortages, rapidly rising natural gas prices, and concerns over global climatic changes thought to be associated with excessive production of carbon dioxide from ever-escalating use of fossil energy use worldwide. In this environment, nuclear electric generation is currently viewed as a key element in addressing these national and global problems and the Department of Energy (DOE) is sponsoring research aimed at developing next generation (Generation IV) nuclear power plant designs that are cost-competitive and are safer and more efficient than present-day technology has produced. Meanwhile, the Nuclear Regulatory Commission (NRC) is moving to reduce regulatory burdens on present and future nuclear plant designs through risk-informed rulemaking processes in order to reduce the costs associated with safe operation of this strategically important industry. Both of these national priorities require the development of new analytical tools capable of effectively integrating the complex physical phenomena associated with the functioning (normal and accident conditions) of next generation nuclear designs.

An LDRD was proposed with its major research objective being the feasibility of applying the DOE's Defense Program's (DP) ASCI nuclear *weapons* systems analysis technology to contemporary safety and design analysis of nuclear *energy* systems and the determination of phenomenological and implementation uncertainties associated with the development of such a technology. An important research component of this project is the evaluation of how to integrate NRC's MELCOR Nuclear Plant System Analysis code and its phenomenological models with the DOE's SIERRA suite of ASCI codes, to create a coupled code system capable of performing safety and design analyses on next generation nuclear plant designs faster and with greater fidelity than is now possible.

The SIERRA parallel computing platform for ASCI codes includes high-fidelity thermal, fluids, and structural codes whose coupling through SIERRA can be specifically tailored to the particular problem at hand to analyze complex multi-physics problems. However, the codes were not developed with advanced reactor design analysis in mind. These tools could possibly also be used for detailed analysis of nuclear reactor design problems; presently, however, the suite lacks several physics modules unique to the analysis of nuclear reactors. Typically, a reactor design process would proceed by using lower-fidelity codes to narrow the design space and then using high-fidelity codes to analyze parts of the reactor system in more detail. We proposed to bridge the gap between initial system design and detailed analysis of components, and provide the needed reactor-specific physics, by coupling MELCOR and the SIERRA tool suite.

A 3 year project was proposed to develop a state-of-the-art analysis code suite for nuclear reactor design and safety. The project proceeded in three steps: 1) evaluate the SIERRA code suite for its current applicability to the analysis of nuclear reactors using one of several possible demonstration problems, and select a demonstration problem to have a concrete example to work with; 2) investigate coupling of the SIERRA codes with MELCOR; 3) apply the coupled codes to a demonstration problem involving a nuclear reactor system, over the three year effort. Each of these steps is discussed below.

1.1. Evaluation of SIERRA capabilities and development of coupling plan - Year 1

During the first year we evaluated several proposed next generation reactor concepts with the objective of identifying those phenomena not presently understood well enough to be modeled in current tools. Advanced reactor designs included Modular High Temperature Gas Reactor designs (MHTGR), the Pebble Bed Modular Reactor (PBMR), and the IRIS advanced Westinghouse design. Problem applications examined included off-normal to severe accident conditions, and ultra-high temperature issues as well as completely new nuclear fuel element designs. A major uncertainty in this stage was the question of physics coupling effects and whether SIERRA tools could be successfully coupled to analyze these couplings. In this stage, we evaluated the feasibility of integrating MELCOR models with the SIERRA code suite. This included evaluation of SIERRA code capabilities and how MELCOR capabilities could complement those of SIERRA for application to advanced reactor analysis.

The result of the first year effort was a determination of the feasibility of the proposed analysis methodology, an identification of critical scientific unknowns or obstacles to the proposed analysis tool, and a plan for developing the advanced tool suite. A spent fuel pool problem was selected as the demonstration problem, and several coupling methodologies were evaluated.

1.2. Coupling MELCOR and SIERRA - Year 2

We proceeded in Year 2 with implementation and testing of the proposed code architectural constructions defined in Year 1 in order to demonstrate the feasibility of the new analysis algorithms and methods. Two candidate CFD (Computational Fluid Dynamic) codes were selected for use in the demonstration problem, and MPI (Message Passing Interface) using an executive program was selected as the coupling approach.

1.3. Demonstration of analysis and design capability - Year 3

In the third year, we proposed to perform an analysis of a demonstration problem for an advanced reactor system. The principal candidates originally identified included: 1) the Pressurized Thermal Shock phenomenon for an advanced light water reactor system, and 2) off-normal and severe accident analysis of a gas cooled Generation IV reactor design known as the Pebble Bed Modular Reactor (PBMR). The demonstration problem finally selected was a spent fuel pool problem. Third year activities did not happen as a result of cancellation of the LDRD at the end of year 2.

2. FIRST YEAR ACTIVITIES

2.1. Reactor Designs Examined

We examined several proposed next generation reactor concepts to identify phenomena not presently understood well enough to be modeled by current system simulation tools. The reactor designs include the Modular High Temperature Gas Reactor, the Pebble Bed Modular Reactor, and the IRIS Westinghouse design. Problem applications included off-normal to severe-accident conditions, and addressed both ultra-high temperature issues and new fuel element designs. A major uncertainty was whether SIERRA could be successfully utilized to analyze physics coupling effects. Present SIERRA models do not treat many key advanced reactor physical phenomena, for instance boiling and multiphase flow, aerosol transport and behavior, etc. There is also a limitation on how complex a system can be analyzed as a finite element problem: although parallel computing has extended the level of complexity possible considerably, present computing capability is still far short of that required to mesh up a reactor core, much less an entire reactor system. We therefore evaluated the feasibility of integrating MELCOR system level models with SIERRA as an approach. The evaluation was to determine how SIERRA and MELCOR capabilities could complement each other for application to advanced reactor analysis. The result of this evaluation was a determination of the feasibility of the various proposed analysis methodologies and a plan for developing the advanced analysis tool suite.

2.2. Demonstration Problems Examined

We evaluated possible demonstration test problems with regard to what physical quantities would be coupled between MELCOR and the high-fidelity code(s), and at what fidelity (finite element node, surface set, etc). The evaluated problems were:

1. Lower head molten pool with crust formation. This problem would use MELCOR to set up the initial and boundary conditions of a molten pool and GOMA[1] (predecessor of ARIA, an ASCI code in the planning stage at the time) to calculate convection and heat transfer in the pool. GOMA models were evaluated for application to the molten pool problem. In discussions with GOMA developers, it was discovered that there are currently no eutectics in GOMA, although there are hooks for such a model. This would mean that the very rudimentary eutectics model in MELCOR would have to be coupled to GOMA at the GOMA cell level. Coupling a property routine from MELCOR into an ASCI code using tight coupling is not a first choice for a demo problem, as this approach does not use much of MELCOR’s capabilities and amounts to adding property routines to GOMA.

2. Pressurized thermal shock (PTS). This would use MELCOR for thermal conditions in the vessel and two-phase flow of the coolant, and the structural response code PRONTO[2] (predecessor of the PRESTO ASCI code) for the structural response of the vessel break.

3. Spent fuel pool fire. This would use MELCOR for the fuel pin behavior, including temperature and clad oxidation rates. FUEGO (an ASCI fire code) would provide convective gas flow using the fuel pin temperatures and clad oxidation rates as boundary conditions. FUEGO would also handle phenomena associated with a jet fuel fire. FUEGO models were evaluated for application to the fuel pool problem. Transfer of parameters from MELCOR to FUEGO would be done via user functions in FUEGO.

4. Heat transfer and convective flow around pebble bed reactor fuel. MELCOR would provide overall system conditions, CALORE (a heat transfer code) and FUEGO would calculate the thermal response of the fuel and coolant flow around the fuel.

We reviewed several technologies for possible use in coupling MELCOR and ASCI codes. One method is to use the DAKOTA (Design Analysis Kit for Optimization and Terascale Applications) executive code. DAKOTA can be used to control MELCOR and ASCI codes together, plus synchronize the code coupling. Transfer of parameters from MELCOR to ASCI codes would most likely be done via user functions in the ASCI codes. This approach requires that either DAKOTA/MELCOR/ASCI codes be running on the same platform or that jobs can be dispatched from the machine running DAKOTA. The DRM (Distributed Resource Management) project is also addressing the problem of running on distributed platforms.

Another method would be to use Entero, a system simulation environment project currently under development[3]. This option would have to be used in conjunction with DRM to use JANUS but could be used if networked workstations were used as the computing platforms. PVM[4] is also a solution for machines other than JANUS (JANUS doesn’t run PVM).

We evaluated a PVM approach which couples MELCOR and RELAP5, a finite difference high-fidelity reactor code. The coupling uses an executive program to control the PVM master and remotes on different networked machines.

The NASA Numerical Propulsion System Simulation project was evaluated for ideas.[5,6] The two referenced papers discuss the problems associated with coupling multifidelity models of flow fields. The principal conclusion of the papers is that coupled flow fields can be numerically unstable. This suggested that coupling MELCOR and ASCI code-generated flow fields was not a good idea for a first test problem, and that using a single flow field from one or the other was an easier approach. The flow field could then be coupled to other physics models, such as heat transfer or structural response, without as much danger of causing numerical instability.

The demonstration problem selected from those was the spent reactor fuel pool problem. The final selection of coupling methodology was deferred to Year 2.

3. SECOND YEAR ACTIVITIES

3.1. Selected Demonstration Problem

The demonstration problem selected from those evaluated in Year 1 was the spent reactor fuel pool problem. The fuel pool would be assumed drained of water and allowed to heat up from decay heat in the fuel. The problem would be split to use MELCOR for the fuel pin behavior, including temperature and clad oxidation rates, and a CFD code would provide convective gas flow using the fuel pin temperatures and clad oxidation rates as boundary conditions.

We proceeded with evaluation of the various proposed code architectural constructions defined in Year 1.

We reached the conclusion that coupling MELCOR to the SIERRA framework codes was not feasible at this time for several reasons, detailed as follows. The most important reason for this conclusion is the SIERRA framework itself. This "framework" is intended to separate the functions of computer implementation of a code and the physics side of code design, by providing common functions for solution, mesh generation, output, etc., and allow coupling of codes inside the framework. Unfortunately, the framework is of use only to finite element codes, provides no "hooks" to allow easy coupling to codes outside the framework, and has a huge learning barrier to incorporating a new code into the framework. Second, it became apparent as we reviewed ASCI code capabilities that many of the codes are in the beta-stage of development. Being in this early development stage has several consequences: lack of documentation; critical physics models being absent; and no developer time for collaboration available for activities outside of ASCI development.

For the above reasons, we investigated the "pre-ASCI" versions of the codes, and other CFD codes available at Sandia. These codes tend to be more established with more models in place. Also, since the older codes are not in development, the codebases are more stable. Codes investigated for possible use in the demonstration problem include MP-Salsa, Vulcan, the "FAA" code,[7,8] a new version of the Coyote/Nachos code,[9] and GILA[10]; these are all 3D CFD codes. MP-Salsa is an equilibrium/transient finite element code; Vulcan is a transient block-structured code; the FAA code, developed to analyze smoke transport in airplanes, uses a body-fitted mesh; and GILA is a transient finite element code. The new Coyote/Nachos code turned out to be at a very early stage of development and was not considered further.

Important criteria in selecting a code include easy mesh generation, stability, documentation, implementation of physics models needed (in this case convection, turbulence, and chemical reaction physics), an active development/user group, and the ability to run on a parallel machine. We selected MP-Salsa as the main candidate and GILA as a backup, because they both included the necessary physics, used standard finite element meshes and generators, and had active support. Vulcan and the FAA code were removed from consideration primarily because of non-standard mesh generation and lack of support.

Investigation first focused on evaluating the CFD codes on simplified problems and on development of coupling algorithms and methods for coupling to MELCOR. In this approach, a set of necessary techniques or methodologies needed before the final problem could be done was defined and simplified problems addressing those techniques were defined. Simplified meshes and test problems for a single fuel bundle in the spent fuel pool were set up to gain familiarity with the CFD codes on this type of problem. The simplified test problem is shown in Figure 1. This is a single fuel rod enclosed in a square channel, with specified inflow and free outflow.

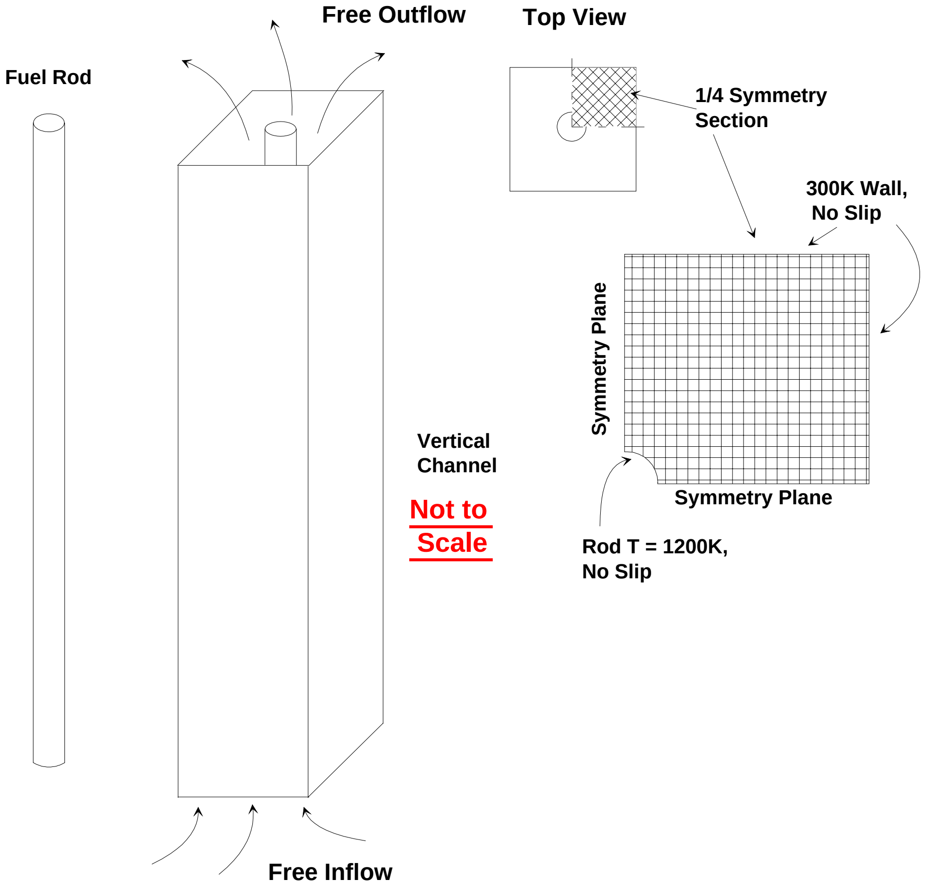

Figure 1. Simplified CFD-MELCOR Test Problem

The selected approach to coupling CFD to MELCOR is oriented around user functions in both codes, with MPI (Message Passing Interface) as the "glue" to communicate between the codes. This approach provides the primary coupling mechanism, and each code sees the other as providing boundary conditions. The problem of coupling between two codes having different spatial fidelities was considered; this involves defining appropriate coarse-to-fine-grid and fine-to-coarse-grid operators for the coupling functions.

3.2. MPI Coupling

There are two widely used message passing interfaces, MPI and PVM, for communications between parallel processes running on a symmetric multiprocessor (SMP) machine or a network of workstations. MPI is extensively supported at Sandia National Laboratories, and PVM is not. However, MPI is better suited for dedicated, massively parallel (MP) SMPs and PVM is better suited for a network of nondedicated workstations that are not always available for parallel processing (e.g., because of network outages or extensive use by other processes). Because of Sandia's investment in dedicated MP SMPs, MPI is the logical choice for message passing interface and is currently the only practical choice at Sandia for running CFD codes in a massively parallel fashion.

There is a problem with the use of MPI, related to the fact that MPI is based on the single program, multiple-data (SPMD) model. This means a single program is executed in each process, but different branches in the program are taken to allow different sets of data to be processed according to the location of a process within the process hierarchy. As a consequence, some MPI implementations do not allow for the use of different executables to be running in parallel in one job, even if the message passing is consistently implemented. If there is no provision for use of different executables, such as through a load file, it would be difficult to couple a number of GILA and MELCOR executables together in parallel in the same job. Fortunately, at least one large computational cluster (CPLANT) and most nondedicated workstation network MPI implementations allow for use of different executables.

In the GILA-MELCOR coupling, we have attempted to use to the extent possible the configuration-controlled coding presently in place in MELCOR to handle the RELAP5-MELCOR coupling. The PVM-based implementation of the latter allows for a compact, input-driven, CONTROL-function specification of the physical quantities involved in the coupling on the MELCOR side. Part of the compactness of the implementation within MELCOR results from the fact that the details of the coupled data exchange are managed by separate controller software called an "executive." In coupled mode, MELCOR runs as a child process under the executive parent; the executive determines, among other things, the nature and order of data exchanged between the child processes. MELCOR itself does not have the logic to function as the executive and also does not adhere to the SPMD model; that is, one cannot run two MELCOR executables by themselves in coupled fashion. (Note that two identical MELCOR processes, with no internal branching based on process hierarchy to break the symmetry, would have no way to determine which process should be the first to send information to the other.) Since this branching is typically extensive, its absence allows for a compact implementation of the coupling, i.e., one that is localized to a handful of MELCOR subroutines.

In order to be able to couple MELCOR and GILA within the Sandia environment, we adopted the approach of using an executive, similar to the PVM based executive for the RELAP5-MELCOR coupling, but based on MPI. This would require also translating PVM calls to MPI calls within MELCOR, and tailoring the MPI executive to the GILA-

MELCOR coupling. In a coupled calculation, we would run three different executables in parallel: the MPI executive, GILA, and MELCOR.

In order to develop the MPI executive, we decided to proceed in two steps. The first was to do more-or-less straightforward translations of the PVM executive for the RELAP5-MELCOR coupling and of the PVM coding within MELCOR. This would allow us to test the MPI-translated versions against a previously published MELCOR-MELCOR test problem[11] run with the PVM executive. This step has been completed, with good agreement between the MPI and the PVM versions. The next step would be to modify GILA with the additional MPI calls to deal with the coupling to the MPI executive and to MELCOR. This latter step was not completed before termination of the project.

3.3. GILA Tests

The approach taken for GILA-MELCOR coupling from the GILA side was again by using simple problems that addressed single aspects of the overall problem. A test was done to get GILA to exchange data via MPI with an executive program, and a simple fluid flow-heat transfer test problem was defined for basic MELCOR-GILA coupling.

Conceptually, MELCOR would supply the heat flux/unit area at node point locations from GILA. This would correspond to evaluating the heat flux on each interface face of a MELCOR control volume, then locating the GILA nodes on that face and then passing the heat flux. GILA would return the temperature that should be specified on that face during the transient solution with MELCOR. This would be explicitly coupled in time, so even for steady problems we would use a false transient to get the coupled solution. The interchange of data would be controlled in time by the "mpiexec" program.

The basic fluid flow-heat transfer test problem as seen from the MELCOR side is a 1m long vertical slab with fluid flow on one side. There are 10 vertical nodes, each with an associated control volume. The wall slab is 10cm thick with 10 finite difference nodes through the slab, each 1 cm thick. On the GILA side, the flow channel would be meshed up as a fluid flow problem with constant mass inflow/constant pressure outflow boundary conditions, and the wall slab seen as a temperature boundary condition.

The slab outside boundary condition is constant at 500K. The inside (facing the fluid) is convective with a high heat transfer coefficient (10^8 W/m^2 K), so effectively the fluid temperature boundary condition is the slab surface temperature. The initial temperature is 300K. The depth of the problem is 1m.[1]

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[1] In the coupling to GILA, MELCOR sends the fluid code the surface heat flux for each vertical node as the variables HS-QFLUX-ATMS-L.10101 through HS-QFLUX-ATMS-L.10110, in W/m2. MELCOR receives the fluid temperature as CFVALU.501 through CFVALU.510 in K.

3.4. MELCOR-MELCOR Test Problem

The purpose of this test problem was to demonstrate and verify the operation of the coupling on the MELCOR side using PVM. In this problem, a MELCOR process is used for the fluids side of the problem also, whereas in the final test problem, this side would be computed using a CFD code. A MELCOR-MELCOR coupled run was executed to test MELCOR exchange capabilities[12]. What was done was to define the test problem in MELCOR, split the test problem along reasonably defined lines, and compare split results to unified results obtained by doing the entire test problem in one MELCOR process. The scenario (see Figure 1) consisted of a single burnt, cooled PWR fuel rod in a spent fuel pool (SFP) subjected to open-air conditions (loss of coolant in SFP). The rod continues to produce decay heat (243.5W). Air is allowed to naturally convect around the rod. Heat-up and oxidation is allowed.[2]

The following discussion details the procedure used to make MELCOR coupling calculations. It is included here for future reference.

3.4.1. COR modeling & methodology

MELCOR uses the COR package to model the fuel region of a nuclear reactor. For this project a single fuel pin was modeled using the COR package. The COR package along with the CVH package are used to model the fuel pin and surrounding air, while the HS package modeled the vertical channel. The COR model is divided into 10 axial levels and 1 radial ring. The first axial level is a support structure. Although this structure is 0.43181m in height, its mass is minimal and therefore does not affect the fluid flow or heat transfer; its only purpose is to keep the fuel pin standing (a MELCOR computational peculiarity). Axial Levels 2 through 10 contain the fuel pin and air. The fuel pin is modeled with the COR package while the air is modeled with the CVH package. Levels 2 and 10 are 0.4318m in height, while Levels 3 through 9 are 0.4608m in height. Levels 2 through 9 were set at 500K while Level 1 was set to 300K. For COR input, data from the Sequoyah Nuclear Power Plant, a Westinghouse PWR, is used on a single-fuel pin basis. A decay heat of 243.5 W and a flat power distribution were applied.

The CVH input for the associated COR input consists of one control volume per COR cell. Each control volume is filled with air at 300K and 1 bar. There is a flow path to and from each control volume as can be seen in Figure 2. From CV110 there is a flow path to CV900, which is the environment. From CV101 there is a flow path to CV900.

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[2] It must also be noted that this scenario uses MELCOR_RH.exe, a MELCOR version including PVM. It also uses a control function argument and a patch that may or may not be in the final version of the code. The new argument is COR-EBND-RAT.ia which passes the radiation from the pin to the canister. The patch allows for calculation of non-zero control volume flow variables by entering a flow area on the CVnnn03 card.

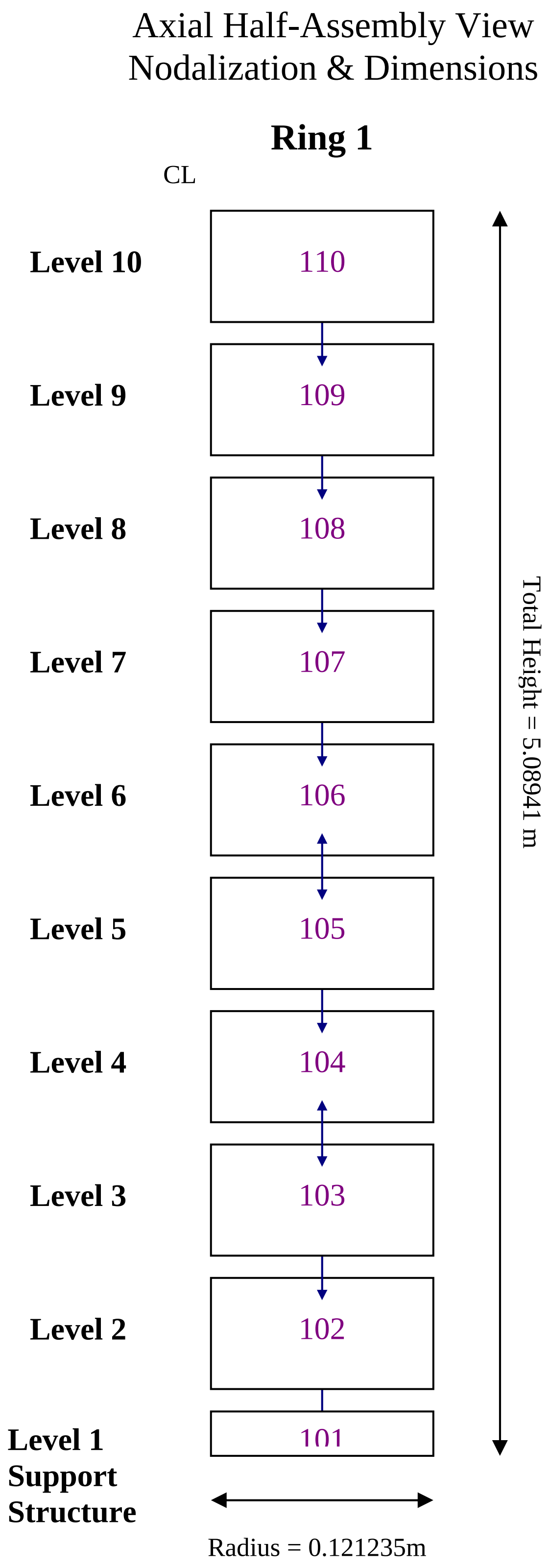

Figure 2. MELCOR CVH Nodes

3.4.2. Heat Structure Modeling & Methodology

Heat structure input was used to model the steel basket surrounding the fuel pin. The boundary conditions specified in the problem definition were also included in the HS input.

The HS configuration corresponds closely to that of a typical COR HS input; the only heat structures in the model are those that correspond to COR cell. There is a single radial heat structure for each axial level. These radial heat structures model heat transfer by convection and conduction in and within the steel basket. Each radial heat structure is modeled with cylindrical geometry with an inner radius starting at the COR outer radius of 0.121235m and an outer radius of 0.1236734m. Each radial heat structure is thus 0.00224m thick, which is represented by two HS nodes of stainless steel.

Additionally, the problem definition sets the outer basket temperature at a constant 300K throughout the scenario. Unfortunately, heat structures that correspond to COR cells cannot have defined temperature profiles at either surface in the dt/dz model; they must have a COR calculated temperature at one side and a convective boundary condition at the other. In order to compensate for this specious requirement, the outer boundary fluid was specified at a constant 300K by a control function.

A single flat heat structure exists at the bottom of the assembly simply as a COR requirement. There is little conduction/convection from the top of the open basket to the environment, so this heat structure has negligible heat transport characteristics and is added simply because it is a MELCOR modeling requirement.

3.4.3. Split Scenario

The input must be divided along reasonable lines to represent MELCOR and non-MELCOR modeling. The Pin Case (MELCOR), which is modeled with the COR package in MELCOR, models decay heat, fuel properties and temperature, oxidation energy and products. The Fluids Case (MELCOR, to be replaced) is modeled with the CVH and FL packages in MELCOR and models flow properties, velocity, temperature, and mole fractions.

Two cases were run: the “cool” case, with no oxidation of the cladding, and the “oxidation” case, which had a higher rod power to raise the rod temperature enough to start oxidation.

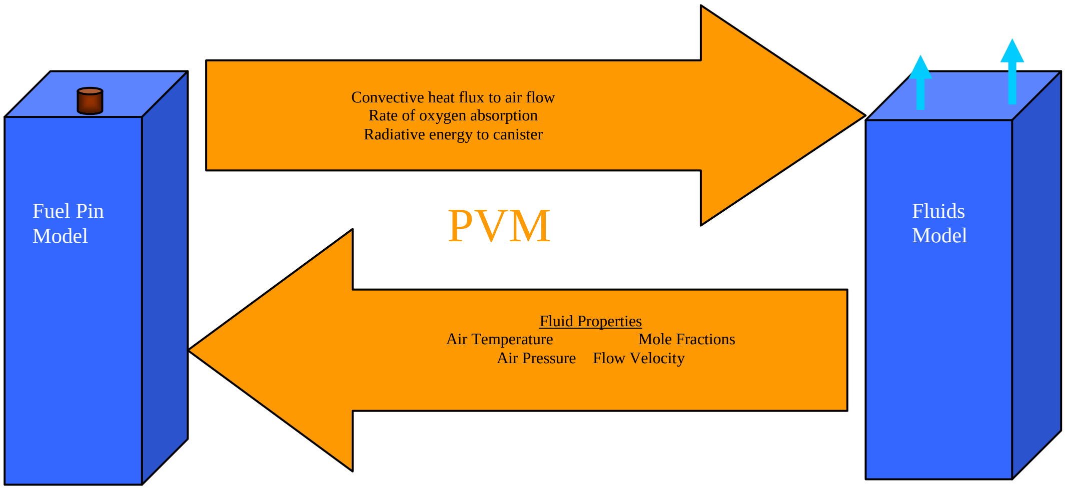

Figure 3. Coupling Information Flow

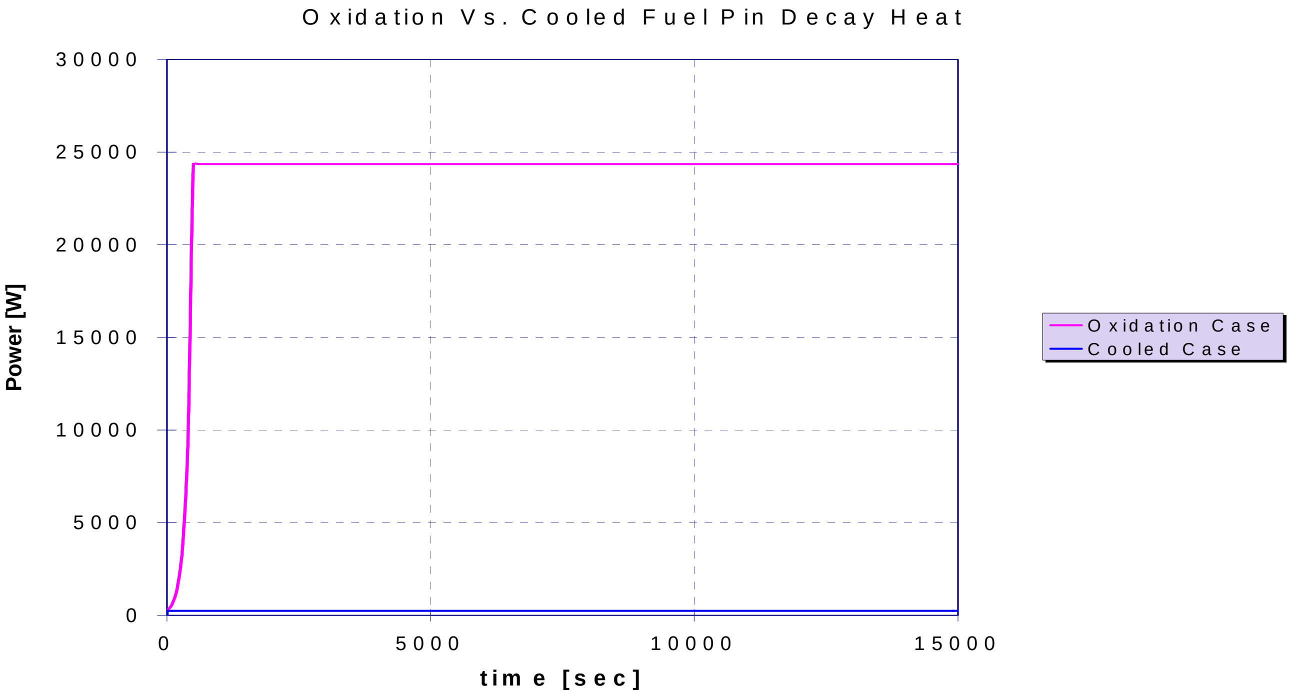

Figure 4. Rod Power for Cool and Oxidation Cases

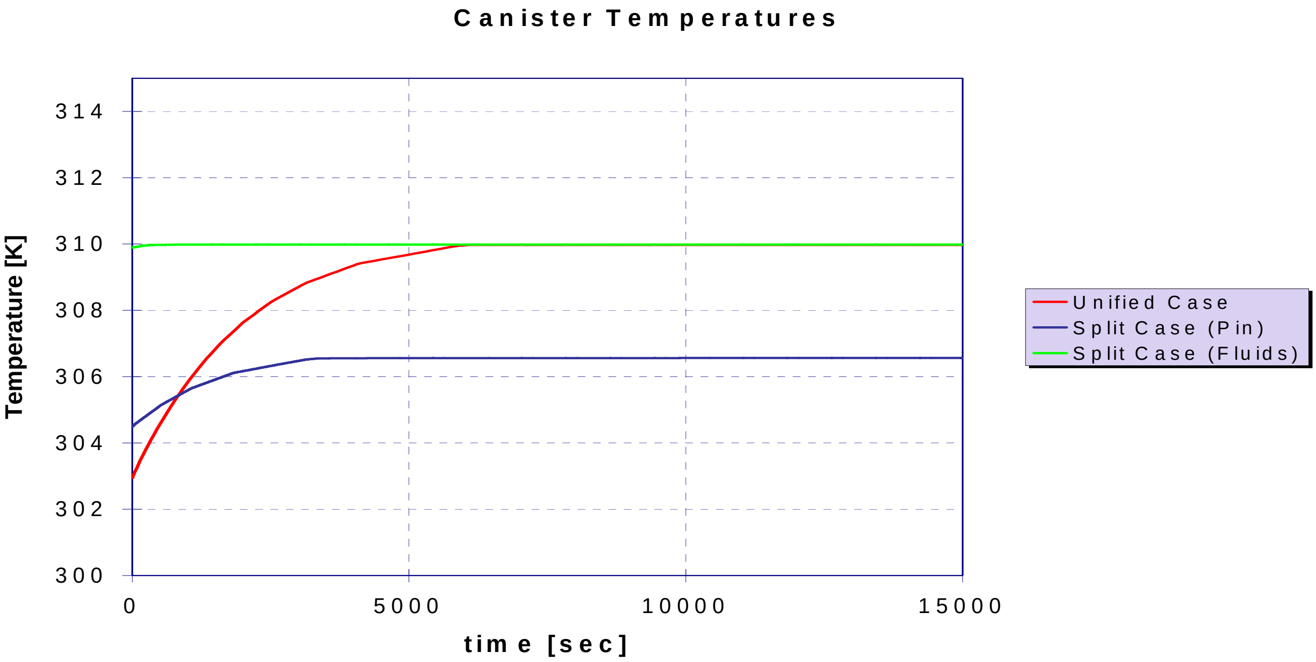

Figure 5. Canister Temperature in Cool Case

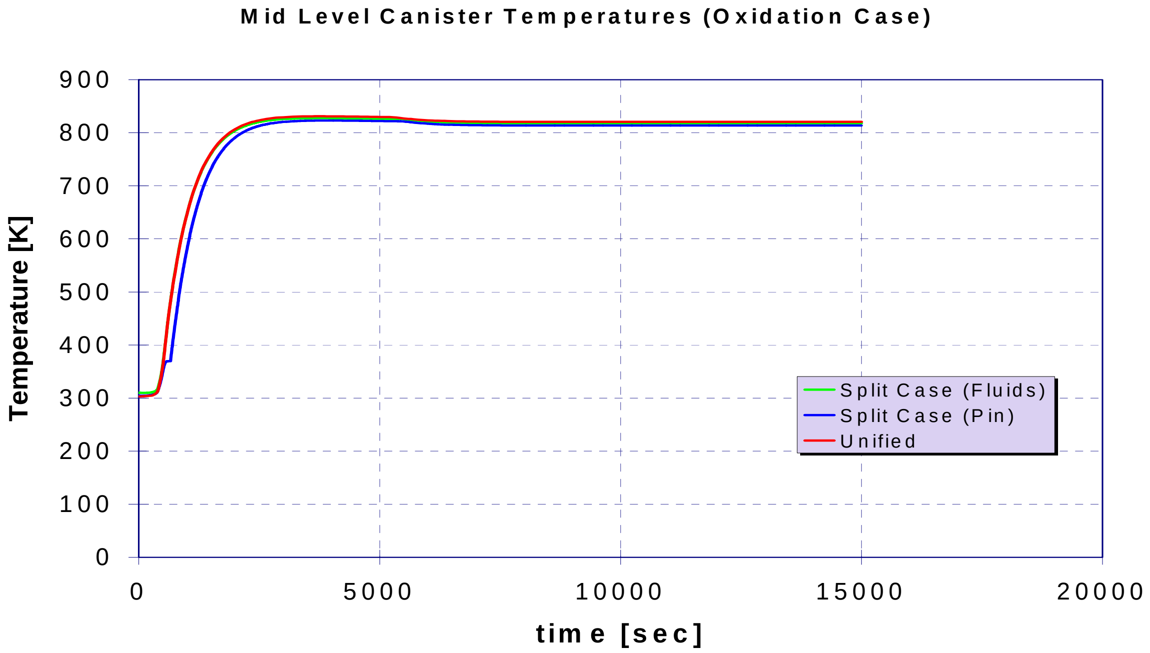

Figure 6. Canister Temperature in Oxidation Case (green and black lines overlaid)

3.4.4. Results of Coupling Test

The results show that the MELCOR side of the coupling interface works. The discrepancies between the unified and split cases are minimal. The most notable difference is about 3.5 degrees Kelvin between the pin canister temperatures and the canister temperatures of the fluids and the unified models for the cool case (see Figure 5). During the oxidation case (Figure 6) the discrepancy is much less.

4. SUMMARY

Several advanced reactor designs and demonstration problems of interest to the reactor community were investigated, along with possible approaches to the problems using coupled MELCOR/SIERRA codes. A spent fuel pool problem was selected as the demonstration problem to use as a concrete example.

We reached the conclusion that coupling MELCOR to the SIERRA framework codes was not feasible at this time for several reasons, detailed as follows. The most important reason for this conclusion is the SIERRA framework itself. This “framework” is intended to separate the functions of computer implementation of a code and the physics side of code design, by providing common functions for solution, mesh generation, output, etc., and allow coupling of codes inside the framework. Unfortunately, the framework is of use only to finite element codes, provides no “hooks” to allow easy coupling to codes outside the framework, and has a huge learning barrier to incorporating a new code into the framework. Second, it became apparent as we reviewed ASCI code capabilities that many of the codes are in the beta-stage of development. Being in this early developmental stage has several consequences: lack of documentation, critical physics models being absent, and no developer time for collaboration available for activities outside of ASCI development.

As a result of the problems with the SIERRA suite, we investigated more established “pre-SIERRA” codes for use with MELCOR.

Several candidate CFD codes were evaluated for possible coupling to MELCOR, the final ones being MP-Salsa and GILA. The one on which the most work was done was GILA. Coupling of GILA to an executive program was demonstrated, and coupling of two MELCOR programs running the fuel rod/channel and the fluids parts of the simplified test problem was demonstrated. A MPI-based version of the original PVM executive program was developed.

Coupling was demonstrated with the simplified test problem using two MELCOR processes. The PVM routines in MELCOR have been modified to include MPI calls. Substantial progress was made in coupling MELCOR with GILA.

While more code coupling experimentation was possible, significant progress toward our goal of demonstrating high fidelity and rapid design analyses of next generation reactors was not feasible. Further work on coupling was discontinued due to termination of the third year of the project. The completed work of a MPI-based PVM executive has increased the fidelity and capability of MELCOR and benefited our severe accident analysis program.

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